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CCR Center for Computing Research

Kokkos Evolution: Task-DAG and Back-ends

DOE COE Performance Portability

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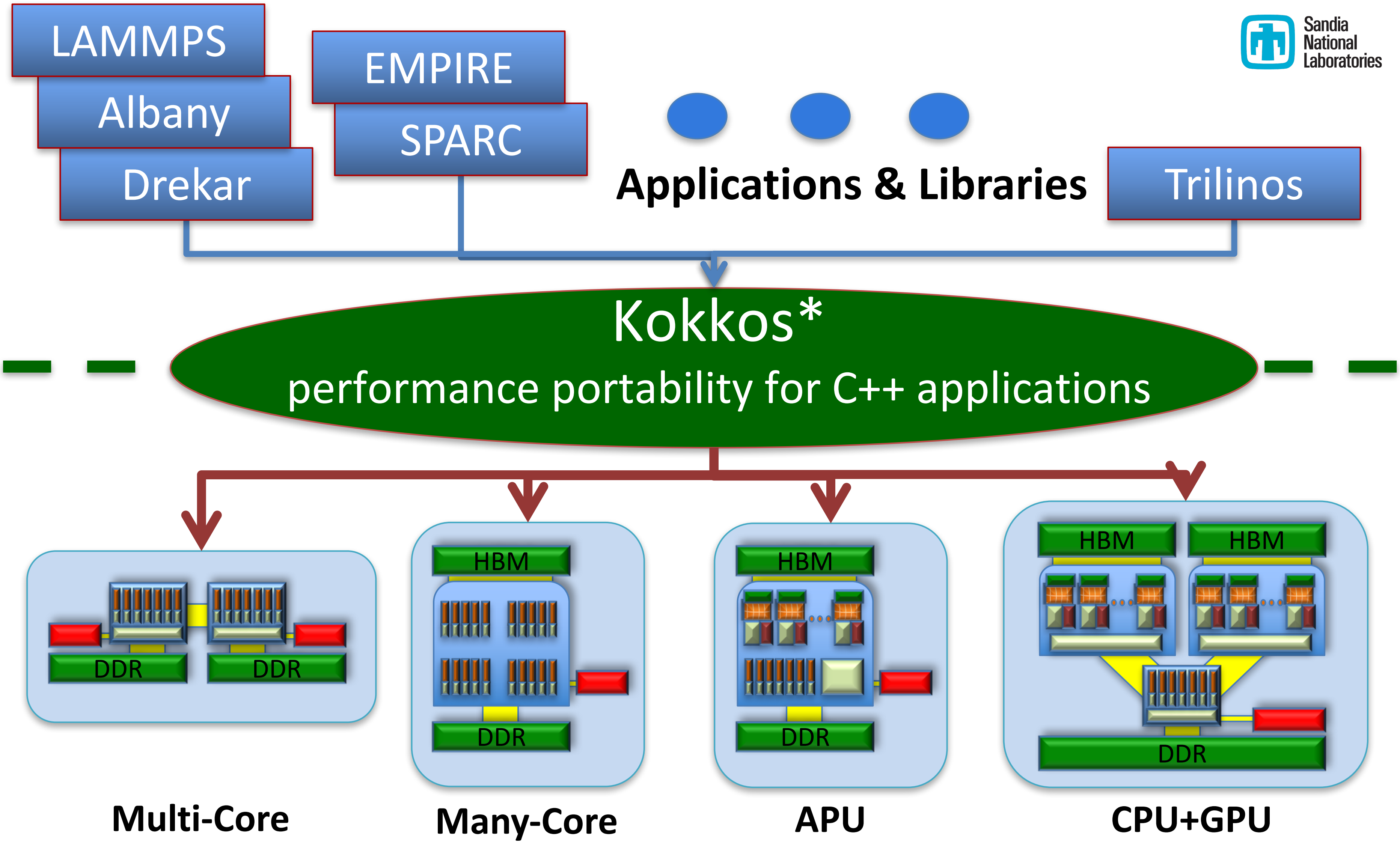


*κόκκος Greek: “granule” or “grain” ; like grains of sand on a beach

Part 1: Kokkos’ Back-ends

- **Map algorithms and arrays to underlying NGP node architecture**
  - **Productive, performance-portable abstractions / programming model**
  - **Map onto architecture’s best programming mechanism: CUDA, OpenMP, ...**
  - **Abstractions and programming mechanisms are evolving**

Part 2: Kokkos’ Task-DAG Pattern/Policy

- **Previously only data parallel patterns / policies**
  - **parallel_for, parallel_reduce, parallel_scan patterns over range policy [0..N)**
  - **Optional hierarchical thread team policy to maximize available parallelism**
- **New directed acyclic graph of tasks parallel patterns / policies**
  - **Tasks: Can be <u>heterogeneous</u> collection of parallel computations**
  - **DAG: Tasks may have acyclic execute-after dependences**
  - **Dynamic: Tasks can be spawned within executing tasks**

FY17-18 evolution of Kokkos' Back-ends

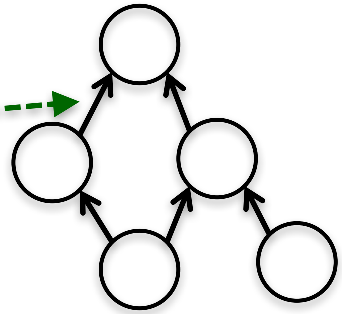
- **OpenMP for CPU and KNL+**
  - Require OpenMP 4+ for proper granularity of thread-binding
  - Compatibility / interoperability with nested parallel regions
    - Continue optional use of hwloc to choose performant sizes for nesting
  - Leverage matured OpenMP 4+ features
    - Scheduling, loop collapse, customized reductions, ...
  - Strategy for performant AMT / Kokkos / OpenMP interoperability
    - Outcome of collaboration with U-Utah's "Uintah" framework
- **CUDA 9+ for NVIDIA GPU**
  - Proper collectives and controls provided by CUDA thread groups
    - Address warp divergence bug
  - Sub-block thread teams to improve flexibility of hierarchical parallelism
    - Best realized on Volta architecture
  - Full host-device lambda capability with C++17 capture: [=,*this]

FY17-18 evolution of Kokkos' Back-ends

- **C++11 std::thread for CPU and KNL+**
  - **Portability to OS/runtime that does not OpenMP (e.g., Windows)**
  - **Performance comparison with OpenMP**
  - **Research thread synchronization and collectives, runtimes**
- **Backend for ARM (CPU)**
  - **OS/runtime/compiler stack? tbd**
  - **Best thread parallel mechanism: OpenMP, std::thread, ...? tbd**
- **ROCm for AMD GPU; developed by AMD**
- **OpenMP 4.5 offload for GPU**
- **Clang-CUDA for GPU**

Directed Acyclic Graph (DAG) of Tasks

- **Pattern**
  - **Parallel execution of computations (tasks)**
  - **That have "execute after" dependences**



- **Policy**
  - **Scheduling ready tasks**
  - **Updating dependences as tasks complete**
- **Dynamic and Heterogeneous Task-DAG**
  - **Manage tasks' lifecycle – tasks spawned within executing tasks**
  - **Manage tasks' memory – task and workspace allocated/deallocated**
  - **Each task may be a different function (C++ closure)**
- **Static and Homogeneous Work-DAG**
  - **Single function, similar to data parallel patterns**
  - **Predefined DAG of "execute after" work indices:** { k executes-after { i, j, ... } }

Task-DAG Motivating Use Cases

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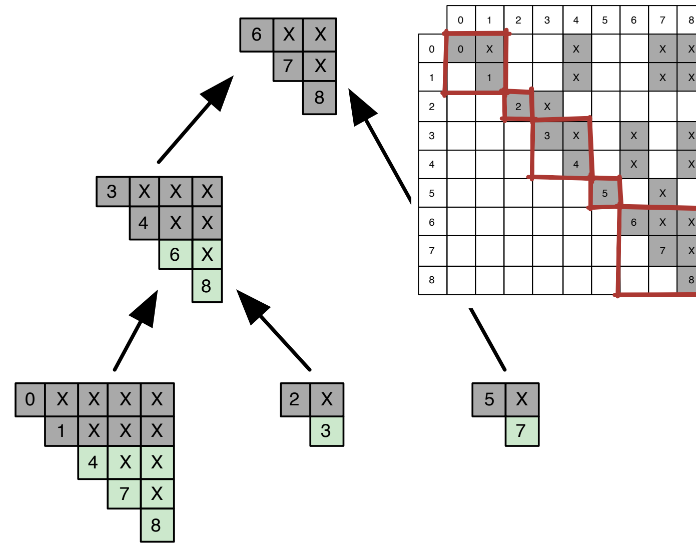
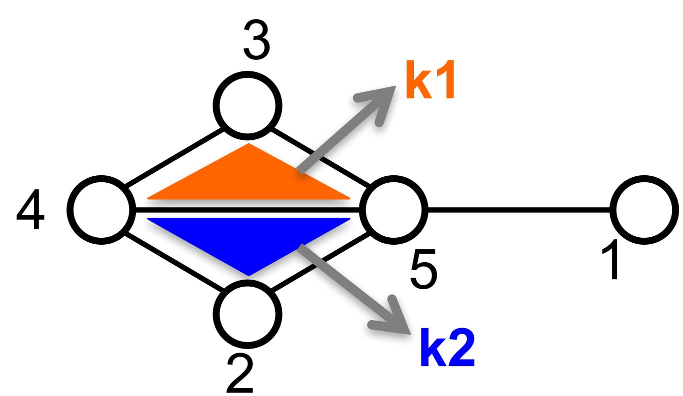
1. Multifrontal Cholesky factorization of sparse matrix

- Frontal matrices require different sizes of workspace (green) for sub-assembly
- Hybrid task parallelism: tree-parallel & matrix-parallel within supernodes (brown)
- Dynamic task-dag with memory constraints
- Matrix computation is internally data parallel
- Lead: Kyungjoo Kim / SNL



2. Triangle enumeration in social networks, highly irregular graphs

- Discover triangles within the graph
- Compute statistics on those triangles
- Triangles are an intermediate result that do not need to be saved / stored
  - Challenge: memory "high water mark"
- Lead: Michael Wolf / SNL



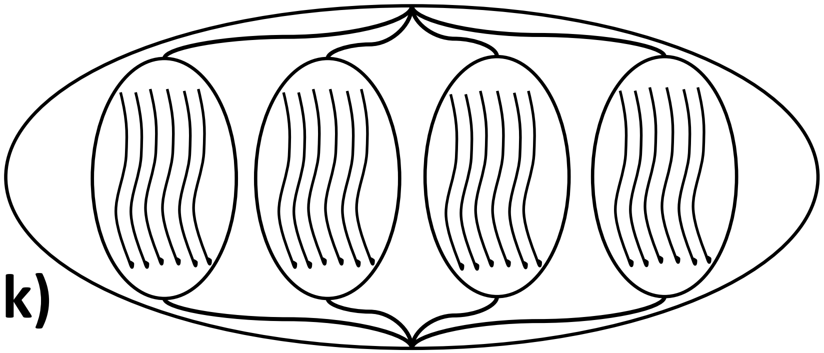
Work-DAG Motivating Use Case

- Neutral Particle Transport via Sweeps
  - Tycho2 mini-application (https://github.com/lanl/tycho2)
  - "A neutral particle transport mini-app to study performance of sweeps on unstructured, 3D tetrahedral meshes."
  - Lead: Kris Garrett / LANL

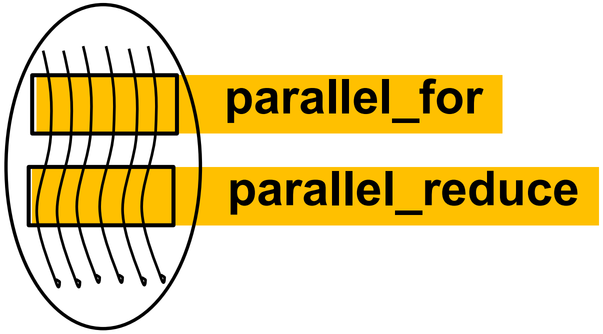
- Tycho2 version using Kokkos Work-DAG
  - All angle sweeps through unstructured mesh in a single DAG
  - Work index: K = angle_index * number_elements + element_index
  - Angle sweeps define work "execute after" dependences
  - Running on CPU and KNL - as of July 27, 2017
  - Next steps:
    - Port data structures to Kokkos for performance portability to GPU
    - Performance evaluation and improvements

Hierarchical, Thread Team Parallelism

- **Shared functionality with hierarchical data-data parallelism**
  - The <u>same</u> kernel (task) executed on …
  - OpenMP: League of Teams of Threads
  - Cuda: Grid of Blocks of Threads



- **Inter-Team Parallelism (data or task)**
  - Threads <u>within</u> a team execute concurrently
  - Data: each team executes the same computation
  - ➢ **Task: each team executes a different task**
- **Intra-Team Parallelism (data)**
  - Nested parallel patterns: for, reduce, scan



- **Mapping teams onto hardware**
  - CPU : team == hyperthreads sharing L1 cache’
  - GPU : team == warp, for a modest degree of intra-team data parallelism

Dynamic Task DAG Challenges

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- **A Dynamic DAG of Heterogeneous Functions (closures)**
  - **Map functions onto a single thread *or* a thread team**
  - **Scalable dynamic allocation / deallocation of tasks**
  - **Scalable and low latency scheduling**
  - **Scalable dynamic creation / completion of execute-after dependences**
- **GPU idiosyncrasies / constraints**
  - **Non-blocking tasks, forced a beneficial "respawn" reconceptualization!**
    - **Eliminate context switching overhead: stack, registers, ...**
  - **Heterogeneous function pointers (CPU, GPU)**
  - **Creating GPU tasks on the host *and* within tasks executing on the GPU**
  - **Bounded memory pool and scalable allocation/deallocation**
  - **Non-coherent L1 caches**

Scalable Memory Pool and Task Scheduler

- **Memory Pool**
  - **Lock-free and low latency via atomic operations**
  - **Large chunk of memory allocated in Kokkos memory space**
  - **From which smaller blocks are allocated and deallocated**
- **Task Scheduler**
  - **Memory pool for tasks' dynamic memory**
  - **Multiple prioritized ready queues**
  - **Per-task execute-after waiting queues**
  - ➢ **Each queue is a simple linked list of tasks**
    - **Lock free push/pop via atomic operations**
  - **Explicitly manage GPU non-coherent L1 cache**
    - **Problem: dynamic allocation/deallocation across GPU processors not automically observed by GPU L1 cache hardware**
    - **Solution: explicitly manage via GPU programmable L1 cache, a.k.a. __shared__**

Memory Pool Performance

- **Test Setup**
  - **10Mb pool comprised of 153 x 64k superblocks, min block size 32 bytes**
  - **Allocations ranging between 32 and 128 bytes; average 80 bytes**
  - **[1] Allocate to N% ; [2] cyclically deallocate & allocate between N and 2/3 N**
  - **parallel_for: every index allocates ; cyclically deallocates & allocates**
  - **Measure allocate + deallocate operations / second (best of 10 trials)**
    - **Deallocate much simpler and fewer operations than allocate**
- **Test Hardware: Pascal, Broadwell, Knights Landing**
  - **Fully subscribe cores**
  - **Every thread within every warp allocates & deallocates**
- **For reference, an "apples to oranges" comparison**
  - **CUDA malloc / free on Pascal**
  - **jemalloc on Knights Landing**

Memory Pool Performance

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	Fill 75%	Fill 95%	Cycle 75%	Cycle 95%
blocks:	938,500	1,187,500		
Pascal	79 M/s	74 M/s	287 M/s	244 M/s
Broadwell	13 M/s	13 M/s	46 M/s	49 M/s
Knights Landing	5.8 M/s	5.8 M/s	40 M/s	43 M/s
apples to oranges comparison:				
Pascal using CUDA malloc	3.5 M/s	2.9 M/s	15 M/s	12 M/s
Knights Landing using jemalloc	379 M/s		4115 M/s	
	thread local caches, optimal blocking, NOT fixed pool size			

- Memory pools have finite size with well-bounded scope
  - Algorithms' and data structures' memory pools do not pollute (fragment) each other's memory

Scheduler Unit Test Performance

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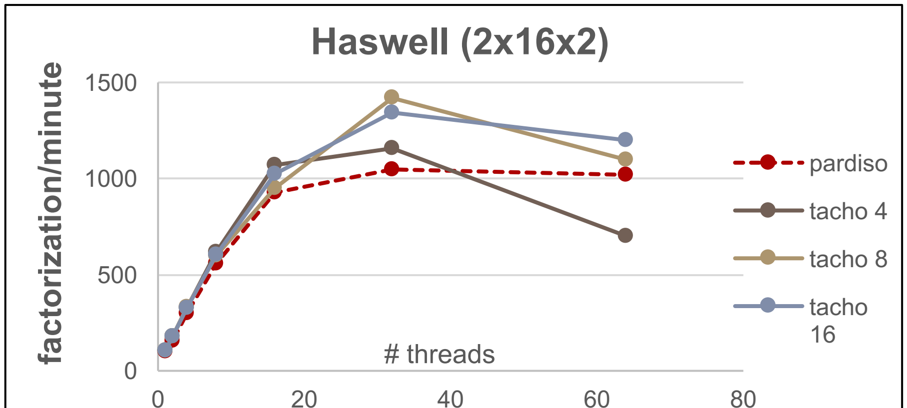
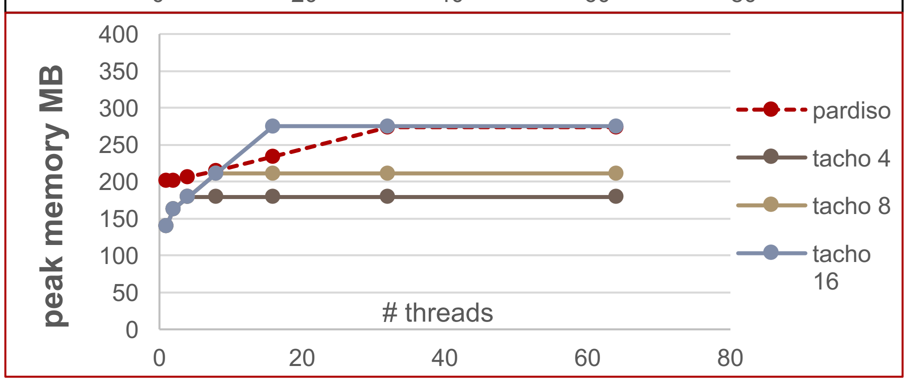
- (silly) Fibonacci task-dag algorithm measures overhead
  - F(k) = F(k-1) + F(k-2)
  - F(k) cumulatively allocates/deallocates N tasks >> "high water mark"
  - 1Mb pool comprised of 31 x 32k superblocks, min block size 32 bytes
  - Fully subscribe cores; single thread Fibonacci task consumes entire GPU warp
    - Real algorithms' tasks have modest internal parallelism
  - Measure tasks / second; compare to raw allocate + deallocate performance

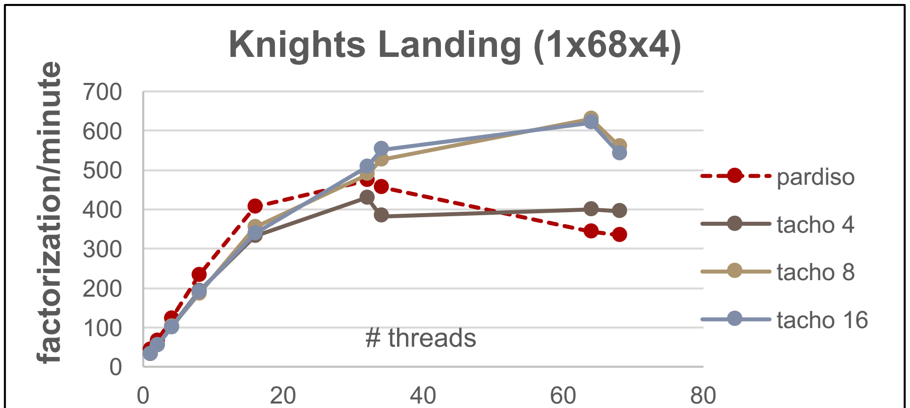
	F(21)	F(23)	Alloc/Dealloc (for comparison)
cumulative tasks:	53131	139102	
Pascal	1.2 M/s	1.3 M/s	144 M/s
Broadwell	0.98 M/s	1.1 M/s	24 M/s
Knights Landing	0.30 M/s	0.31 M/s	21 M/s

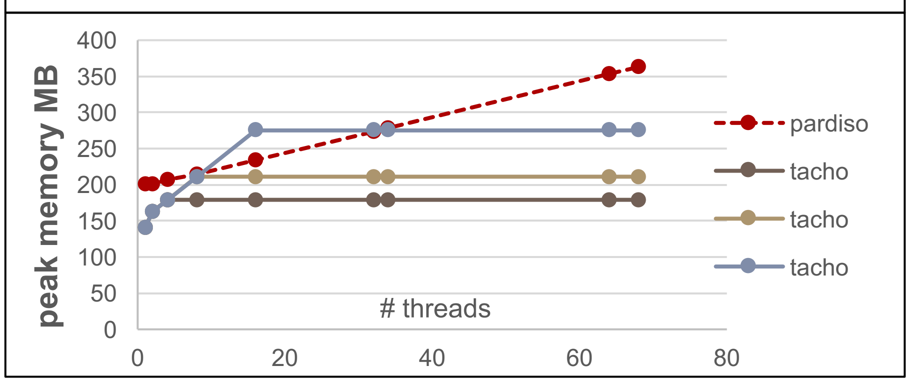
Tacho’s Sparse Cholesky Factorization

- **Multifrontal algorithm with bounded memory constraint**
  - **Kokkos task DAG + Kokkos memory pool for shared scratch memory**
  - **Task fails allocation => respawn to try again after other tasks deallocate**
  - **Test setup: scratch memory size = M * sparse matrix supernode size**
  - **Compare to Intel’s pardiso, sparse matrix N=57k, NNZ=383k, 6662 supernodes**



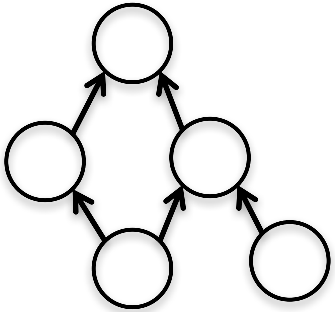






Summary

- Initial Task-DAG capability
  - Portable: CPU and GPU architectures
  - Dynamic DAG of heterogeneous tasks
  - Hierarchical – thread-team data parallelism within tasks
  - Evaluation/improvement underway via sparse matrix factorization mini-app



- Initial Work-DAG capability
  - Portable: CPU and GPU architectures
  - Static DAG of work indices for single work function
  - Evaluation/improvement underway via sweep particle transport mini-app
- Challenges conquered, esp. for GPU portability and performance
  - Non-blocking (non-waiting) tasks ➔ new respawn pattern
  - Lock free, scalable memory pool and scheduler
  - GPU __shared__ memory to address non-coherent L1 cache